COAL LIQUIDS HYDROGASIFICATION: EXPERIMENTS AND MECHANISM

H. N. Woebcke, P. E. Koppel, and P. S. Virk
Stone & Webster Engineering Corporation, P.O. Box 2325, Boston, MA 02107

Experimental data are presented for the hydrogasification of coal-derived liquids at conditions of temperature, pressure and residence time respectively 1200-1700F, 740-1500 psig, and 10-120 s, with hydrogen-to-substrate ratios from 0.8 to 2.0 times stochiometric. The coal liquids originated from hydroliquefaction of Pennsylvania and Wyoming coals; both full range 300-1200F and low boiling 400-650F fractions were employed, all samples being characterized by elemental analysis and NMR spectroscopy. Hydrogasification was performed in a packed tubular flow reactor with sequential effluent quenching and analysis by GCMS to yield information on products from C1(methane) to C14(phenanthrene). Theoretically, it was postulated that the hydrogasification mechanism involves two steps, namely (i) hydrodealkylation of substituted alkyl-aromatics to their nude polynuclear aromatic parent plus gas and (ii) fragmentation of the unsubstituted polynuclear aromatics to progressively smaller aromatic molecules and further gas. The theory predicts that the kinetics of both steps should be governed by the delocalization energy of the aromatic nuclei involved; at the conditions of the present experiments, step (i) should be appreciably faster than step (ii). The experimental data for gas, benzene and naphthalene yields were well rationalized by the theory. Further, the present theoretical framework can be applied to infer hydrogasification behavior of any aromatic feedstock from its NMR analysis, using the aromaticity and ring-breakdowns provided by the latter.